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Modeling the Mixing of High Concentrations of Bidisperse Cohesive Particles in an Inviscid Binder II

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14. ABSTRACT

Funding for this program was provided by the Nanoenergetics Initiative of the Nanoscience and Technology Strategic Technology Thrust.

This document provides the description of model development to simulate the mixing process of cohesive particles with the variety of system parameters to determine their effect on mixtures' homogeneity. The simulation technique known as discrete element model/method (DEM)is used to replace complex mixing procedures with simple plane shear flow with only one species and one size/density being examined. Additional assumptions are made to simplify the binder fluid density and viscosity at this point in the development of the model with great detail planned.

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MODELING THE MIXING OF HIGH CONCENTRATIONS OF BIDISPERSE COHESIVE PARTICLES IN AN INVISCID BINDER II

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Measurement … in Powder and Granular Mixing Paper 409a

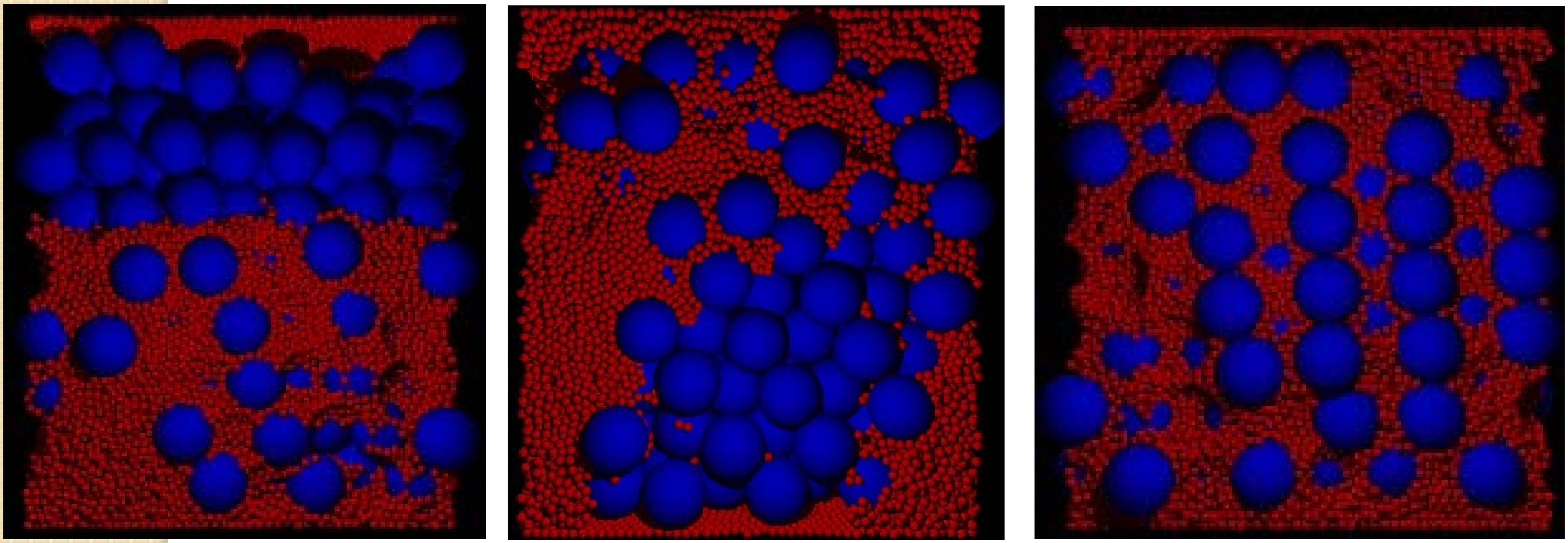
2010 AIChE Annual Meeting

251 B Salt Palace Convention Center, Salt Lake City, Utah

November 10, 2010, 8:30 AM – 8:55 AM

Overview

- Problem: The mixing of differently-sized particles is already difficult due to such phenomena as the Brazil nut effect. Cohesion between particles (e.g. arising from van der Waals, capillary, or electrostatic forces) adds a level of complexity to the mixing.
  - Agglomerates need to be broken up to achieve good mixing
  - Mixing harder to break up agglomerates can lead to greater and faster "unmixing" (e.g. the Brazil nut effect)
  - While the strength of cohesion can often be altered (e.g. via surfactants), the effects of doing so on the mixing process have not been fully explored and quantified, especially when the particles feature a large size range
- To control and maximize the homogeneity of mixtures of cohesive particles, we seek to develop a model that relates a mixture's homogeneity to its components' properties and mixing conditions



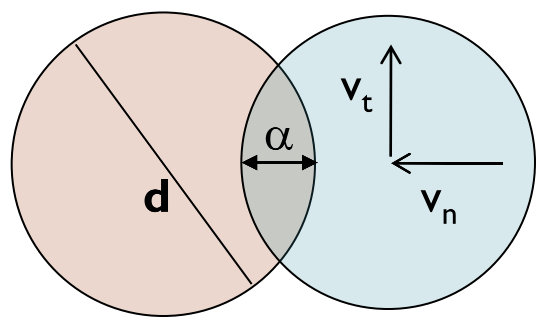
Approach

- Simulate the mixing process of cohesive particles with a variety of system parameters to determine their effect on mixtures' homogeneity
  - Simulation technique: DEM (Discrete Element Model/Method)
  - Replace "complex mixing procedures" with simple plane shear flow
  - Examine only one species, i.e. all particles have same density, Young's modulus, roughness, etc. – only size-segregation and agglomeration due to cohesion will be examined
  - Simplify size and shape distribution by using spherical particles of 2 sizes with 7:1 diameter ratio
    - Individual small particles are able to fit in between packed big particles
    - Homogeneity can have a large effect on total packing fraction
  - Properties to examine
    - Particle cohesiveness , or "stickiness", which can be controlled in real life by surfactants – some or all particles can be altered
    - Shear rate
    - Interstitial fluid (e.g. binder) – buoyancy (fluid density) and viscosity (not discussed here)

DEM simulations*

- The particular DEM code is a modification of LAMMPS, an open-source code from Sandia National Labs
- Every particle simulated as a discrete spherical volume w/ mass
- Particles' positions and velocities calculated by integration of Newton's 2nd law (F = ma)
- Particles are allowed to overlap ("soft") and impose forces analogous to inelastic, frictional springs when they collide

$$F_{normal} = \underbrace{k_n}_{\text{normal spring constant}}\alpha - \underbrace{\eta}_{\text{damping coef.}} v_n$$



$$F_{tan} = \min(\underbrace{k_t}_{\text{tangential spring constant}}\int v_t dt, \underbrace{\mu}_{\text{friction coefficient}} F_{normal})$$

friction coefficient -- limits tangential force according to Coulomb's law of friction

- Cohesion between particles can be simulated by allowing them to attract each other via the van der Waals force

$$F_{van\ der\ Waals} = -\underbrace{A_{eff}}_{\text{Hamaker constant}} d_{eff}/24\underbrace{s^2}_{\text{surface separation}}$$

A is varied for each group of particles to investigate influence of cohesion/surfactants

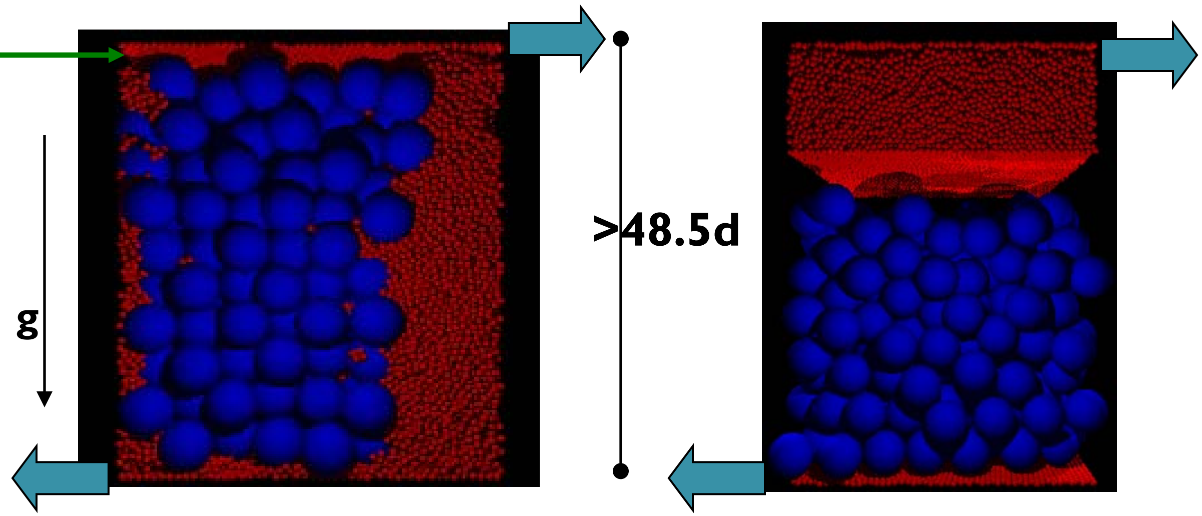
* P.A. Cundall & D. L. Strack, Geotechnique 29 (1979)

Simulation details

45679 small (red) particles of diameter d (~1/4 of solid volume)
367 large (blue) particles of diameter 7d (~3/4 of solid volume)

Big and small particles are initially separated

Ceiling can move vertically to allow for bed contraction and expansion s.t. it applies constant pressure Pd/k = 2.87 × 10^{-4}

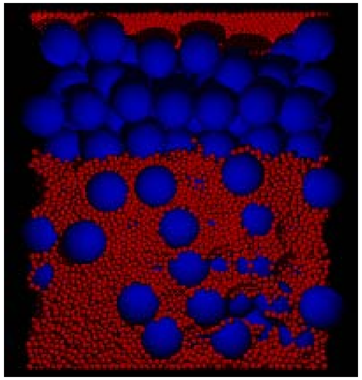


Systems bounded on top and bottom with walls made of small particles which are moved to generate shear
Streamwise & neutral directions are periodic (49d in length)

Interstitial fluid (binder) is not explicitly simulated
It is assumed to fill in all empty spaces and only exerts a buoyant (upward) force on all particles (except the bounds): $F_b = g\rho_b V_p$

Investigating the influence of the binder density

- **Case 1: Particles neutrally buoyant in binder** $\rho_b = \rho_p$
  - **Buoyant forces negate gravitational forces and the resulting gravity-driven segregation (e.g. Brazil nut effect)**
  - **Properties "after long times" (steady-state?) are of interest**
  - **If there is no cohesion, then there will be no driving force for segregation → "best case"**
    - **As cohesion of all particles is increased, segregation should increase**
    - **Increasing shear rate should lead to agglomerates breaking up and small particles getting into gaps between big particles, improving homogeneity**
    - **The effects of altering the cohesiveness of just one group of particles is not immediately apparent**
- **Case 2: Particles denser than binder** $1.8\rho_b = \rho_p$
  - **Big particles will rise to top over time**
    - **How homogeneous do mixtures get before this happpens?**
  - **Unknown if and how varying shear rate and particles' cohesiveness affects homogeneity throughout mixing**
  - **Initial conditions may have strong influence on mixing quality – particles' paths will be affected by gravity**



Simulation dimensionless parameters

When $\rho_b = \rho_p$, particles in effect do not feel any gravitational force (*g* is unimportant), so *g* is not used to scale cohesiveness or shear rate

$$Bo_i^* = \frac{F_{max,i}^{vdW}}{kd} = \frac{A_i d_i}{24kds_{min}^2}$$

"modified Bond number" – dimensionless particle cohesiveness

k = normal stiffness of small particle

$$s_{min} = 2 \times 10^{-5} d$$

minimum surface separation used to prevent van der Waals force model from diverging during collisions Assuming $d \approx 20\mu m$, $s_{min} \approx 0.4nm$, corresponding to typical intermolecular distances

To eliminate the particle size dependence of *Bo and to rescale it to be on average of order unity, we define a scaled modified Bond number:**

$$Bo_i^{**} = 4000 Bo_i^* \frac{d}{d_i} \qquad S = Bo_{small}^{**} \qquad B = Bo_{big}^{**}$$

Shear rate expressed using "scaled stiffness" – dimensionless inverse square shear rate

$$k^* = \frac{k}{\rho_b d^3 \dot{\gamma}^2}$$

Binder density is kept the same among all simulations, unlike the particle density

Order metrics

- **Spatial variance in volume fraction for each particle size**
  - **"Most straightforward" measurement of homogeneity**
- **Total volume fraction**
  - **If well-mixed, small particles fill in gaps between large particles, leading to a high volume fraction**
  - **However, a low volume fraction does not necessarily mean poor mixing**
- **Estimating the average size of clusters of small particles– smaller cluster size means better mixing**
  - **Model has recently been proposed to estimate average cluster size, essentially based on radial distribution function**

$$d_{cluster} = 2\phi^{1/3}\left(L\left(r_{ag}\right)+r_{ag}\right)$$

S. Gallier, Propellants Explos. Pyrotech. 34 (2009)

$$L\left(r\right)=\sqrt[3]{\frac{3K}{4\pi}}-r$$

Besag L-function

J. Besag, J. R. Stat. Soc. B39 (1977)

Maximum value of $L\left(r\right)$ occurs at $r = r_{ag}$ (aggregate radius)

$$K\left(r\right)=\frac{V}{N^2}\sum_{i=1}^{N}\sum_{j\neq i}H\left(r-r_{ij}\right)$$

Ripley K-function (g(r) integrated over space)

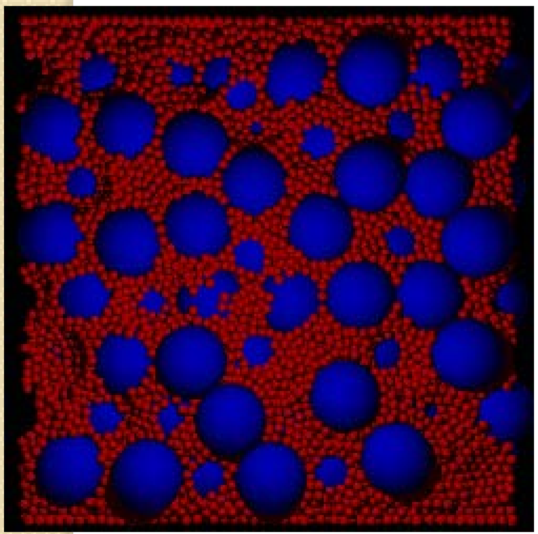
B. D Ripley, J. Appl. Probab. 13 (1976)

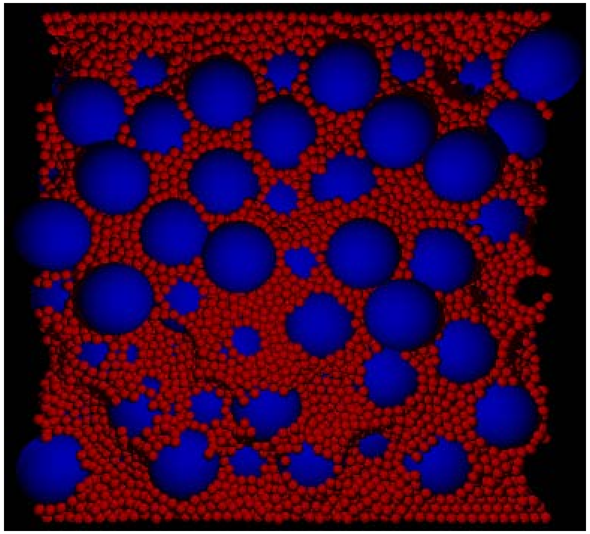
Case 1 Results: Particles neutrally buoyant in binder

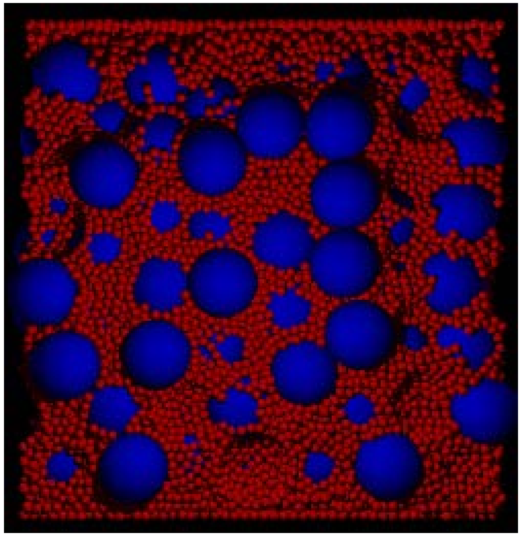
$\rho_b = \rho_p$

***** The results presented in this section are from simulations that have been run for "long times," not necessarily to steady-state *****

As expected, when particles are non-cohesive, the mixtures appear homogeneous







$k^* = 10^9$ $k^* = 10^8$ $k^* = 10^7$

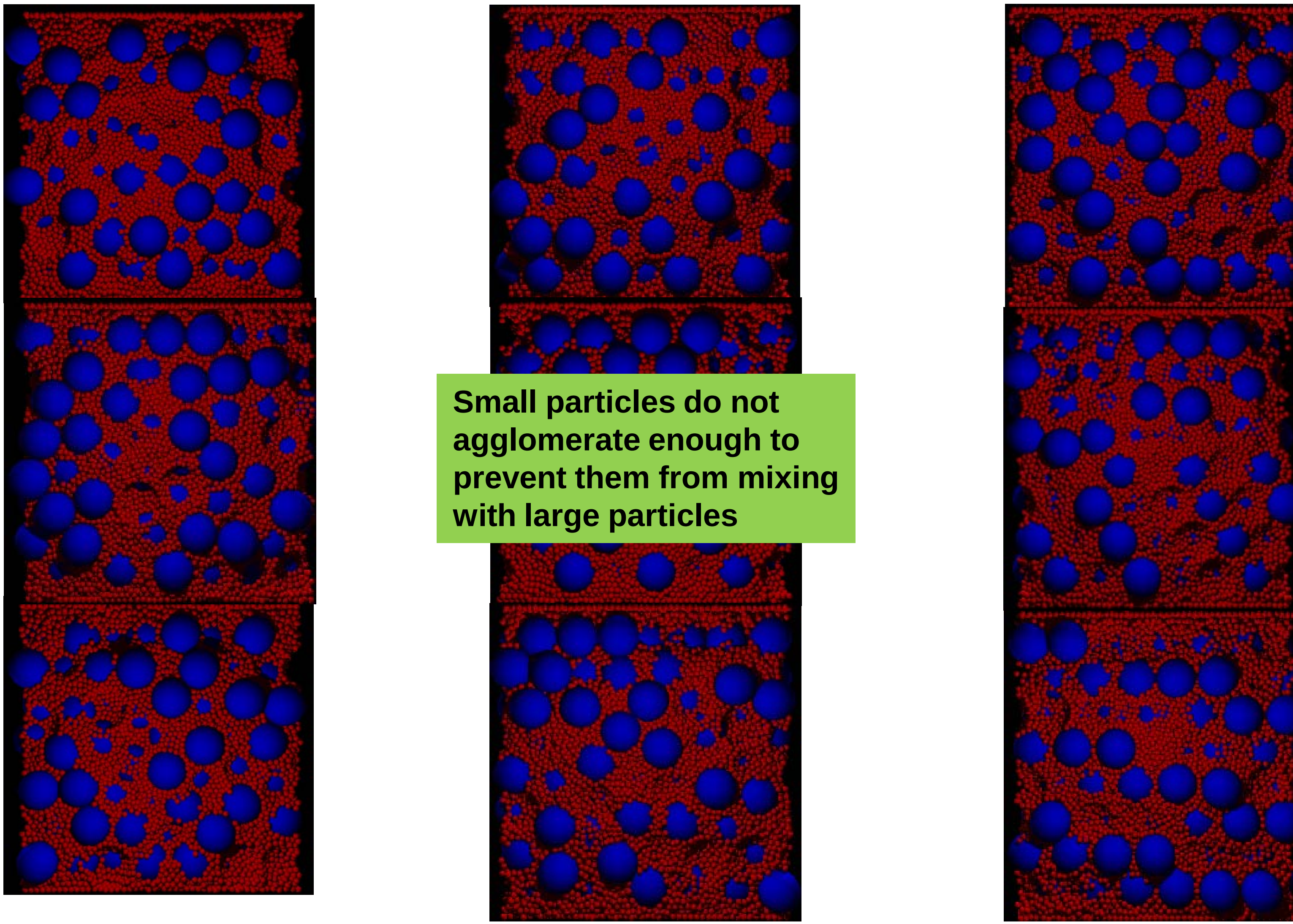
When small particles are not very cohesive (S = 0.1) , the composites also appear relatively homogeneous

B = 0.01 | B = 0.1 | B = 1

k^* = 10^7

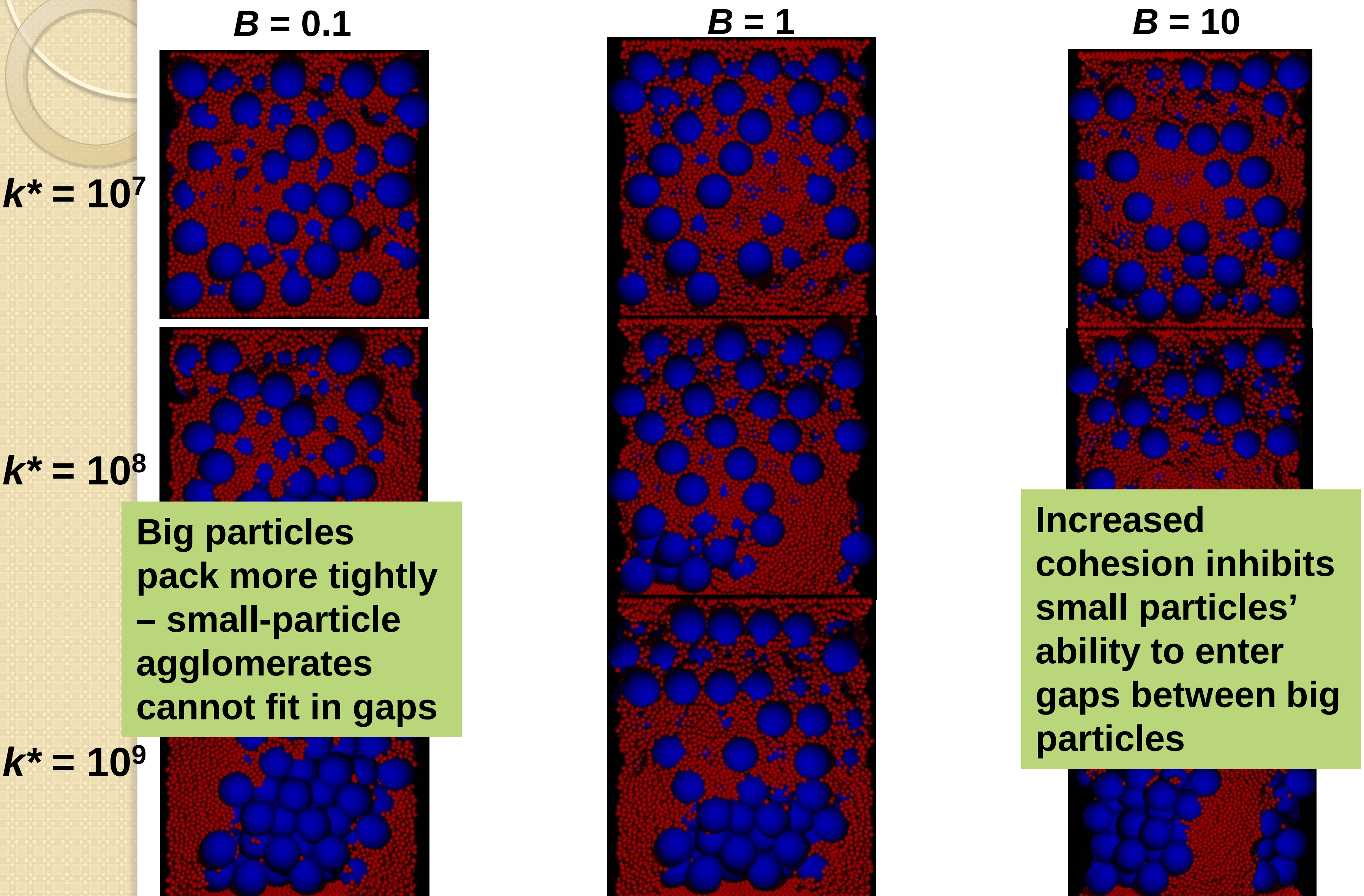
k^* = 10^8

k^* = 10^9

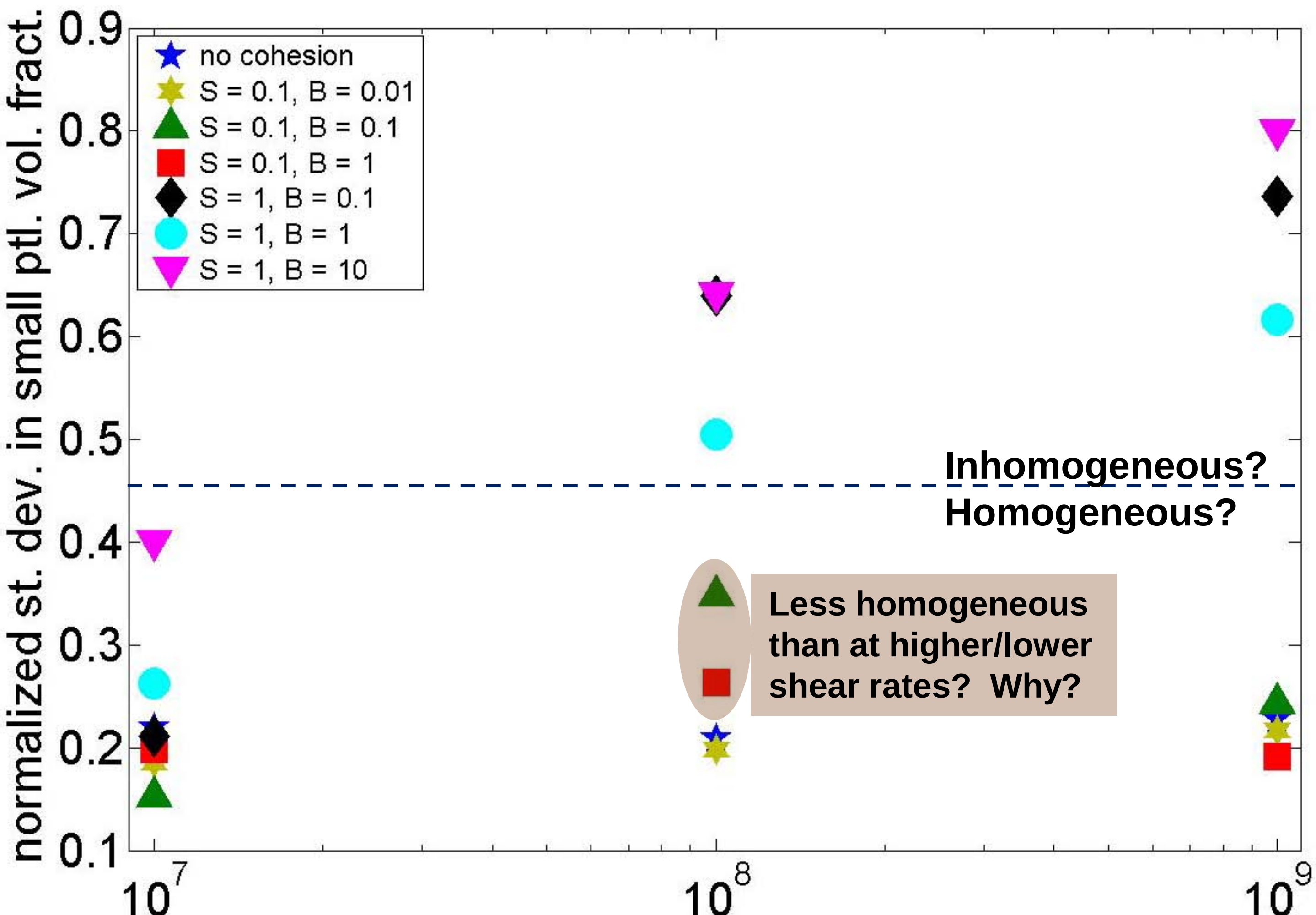


Small particles do not agglomerate enough to prevent them from mixing with large particles

When small particles are more cohesive (S = 1), the composites appear most inhomogeneous at low shear rates and at very high and very low big-particle cohesion

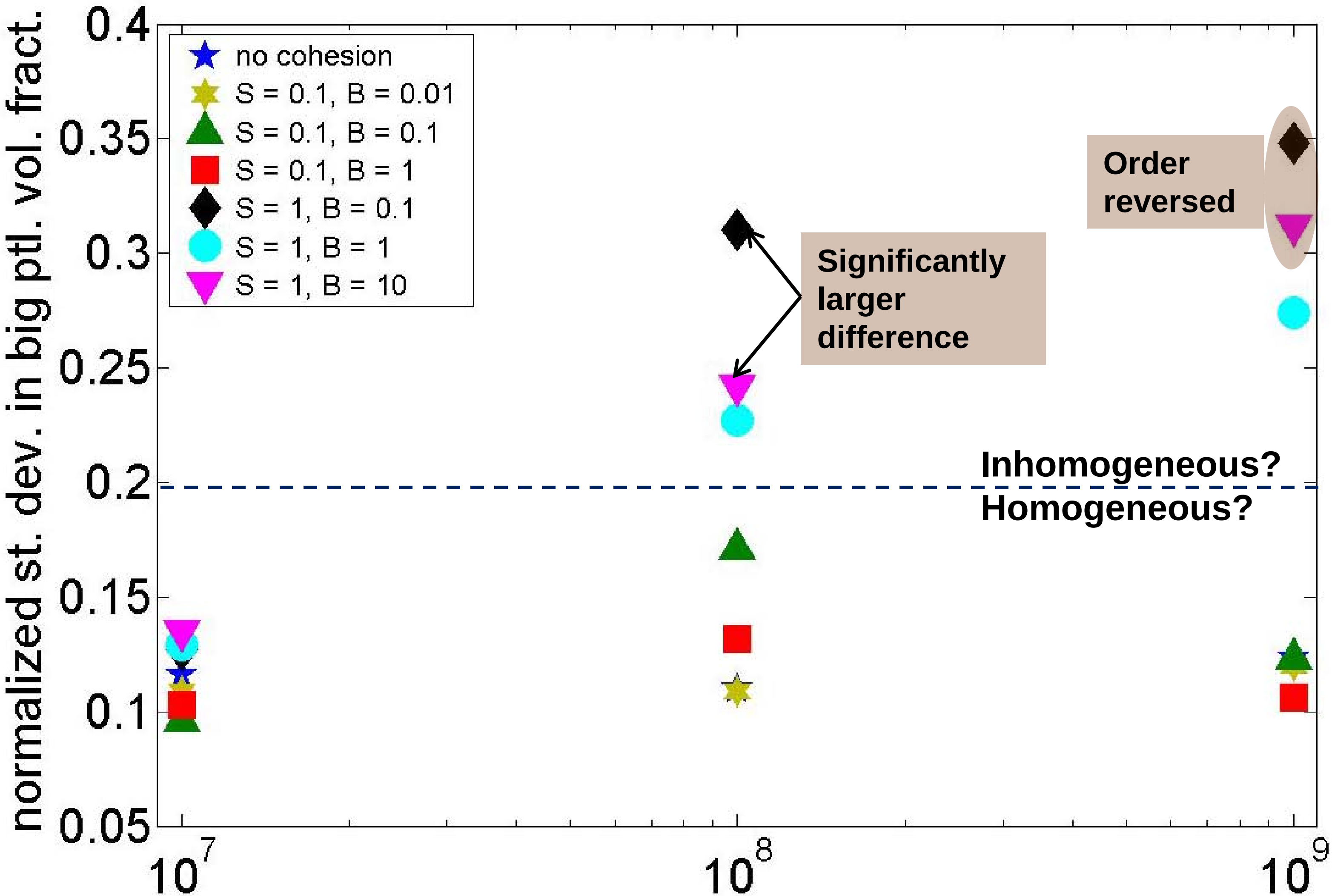


Spatial variance in small-particle volume fraction more or less reflects what was seen in the images

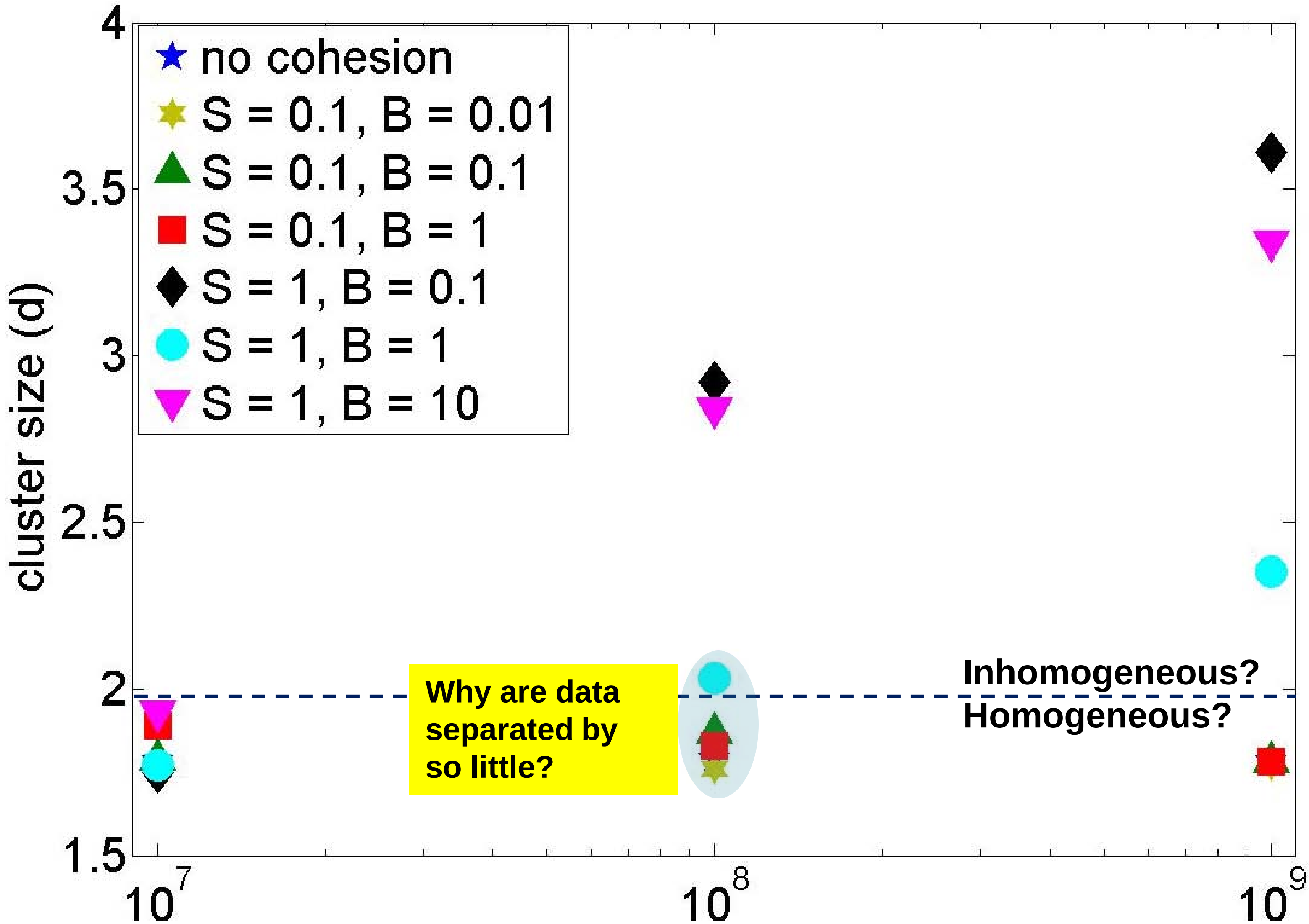


$$k^* = \frac{k}{\rho_b d^3 \dot{\gamma}^2}$$

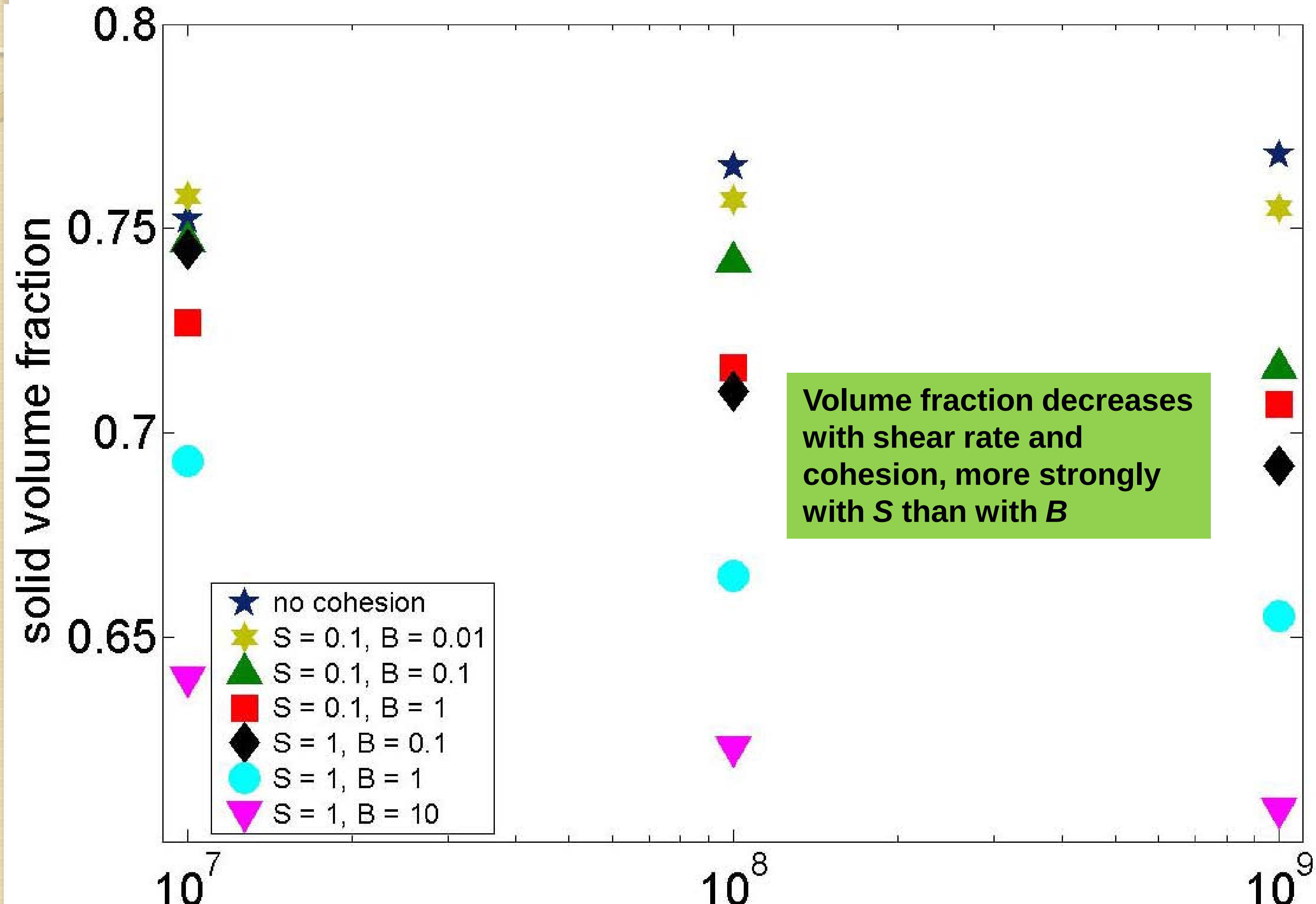
Spatial variance in big-particle volume fraction still reflects images but behaves somewhat differently



Cluster size measurements also reflect mixing quality observed in images but again manifest different behavior



Volume fraction does not capture the homogeneity well but is nonetheless greatly affected by particle cohesion



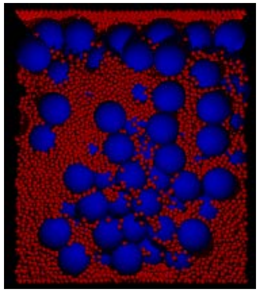
Steady state seems elusive in most cases Should we expect and wait for steady state?

- **Steady state has only been reached under conditions that have produced microstructures that look homogeneous, but not all mixtures that appear homogeneous are at a steady state**
- **If we continue to run these simulations, will the inhomogeneous mixtures eventually become homogeneous or will they stay inhomogeneous?**
  - **If they do eventually become homogeneous, simulations would take unfeasibly long to reach homogeneous states at current pace**
  - **Should the simulations simply be stopped, and if so, when?**
- **The spatial variances in the concentrations of the different particles usually continue to evolve with time well after the total volume fraction and average small-particle cluster size have reached steady state**

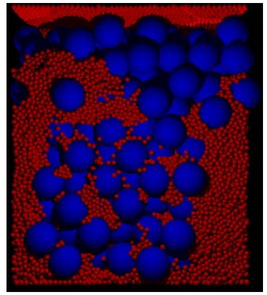
Case 2 Results: Particles denser than binder

$1.8\rho_b = \rho_p$

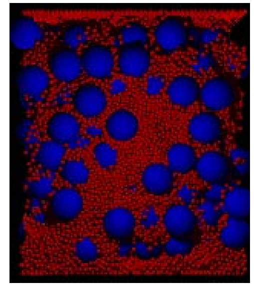
When initially horizontally segregated, large particles generally reach the top before good mixing can be achieved, regardless of cohesion and shear rate



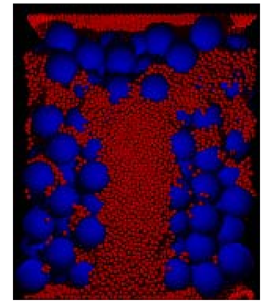
No cohesion
$k^* = 10^7$



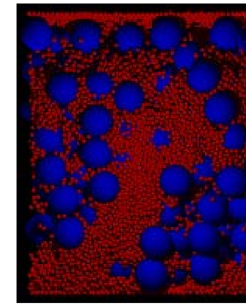
No cohesion
$k^* = 10^9$



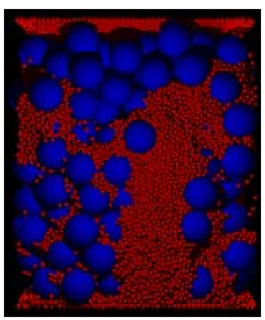
$S = 0.1$
$B = 1$
$k^* = 10^7$



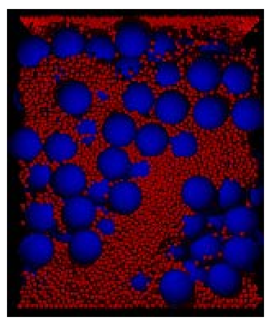
$S = 1$
$B = 0.1$
$k^* = 10^7$



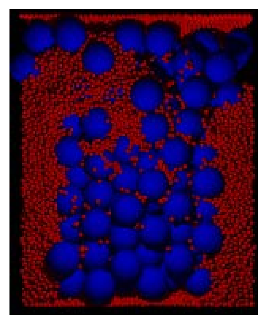
$S = 1$
$B = 0.1$
$k^* = 10^9$



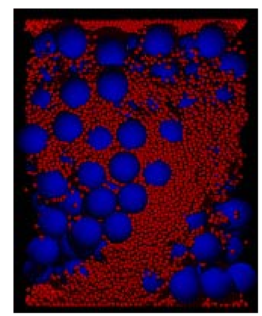
$S = 0.1$
$B = 1$
$k^* = 10^9$



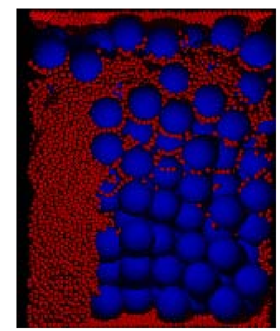
$S = 1$
$B = 1$
$k^* = 10^7$



$S = 1$
$B = 1$
$k^* = 10^9$



$S = 1$
$B = 10$
$k^* = 10^7$

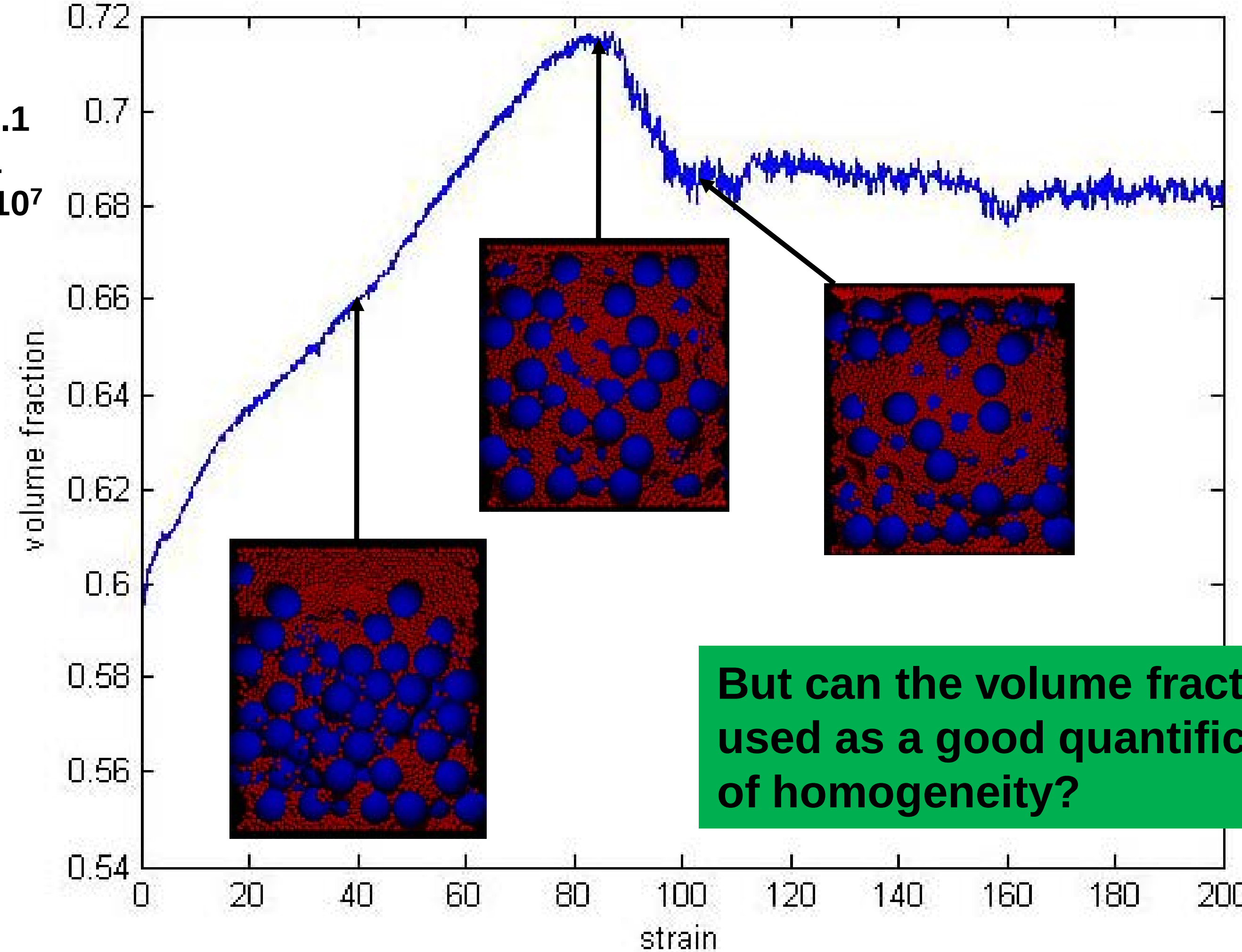


$S = 1$
$B = 10$
$k^* = 10^9$

So we turn our attention to simulations starting with vertically segregated particles

Volume fraction reaches a peak when images show well-mixed and drops off as un-mixing occurs

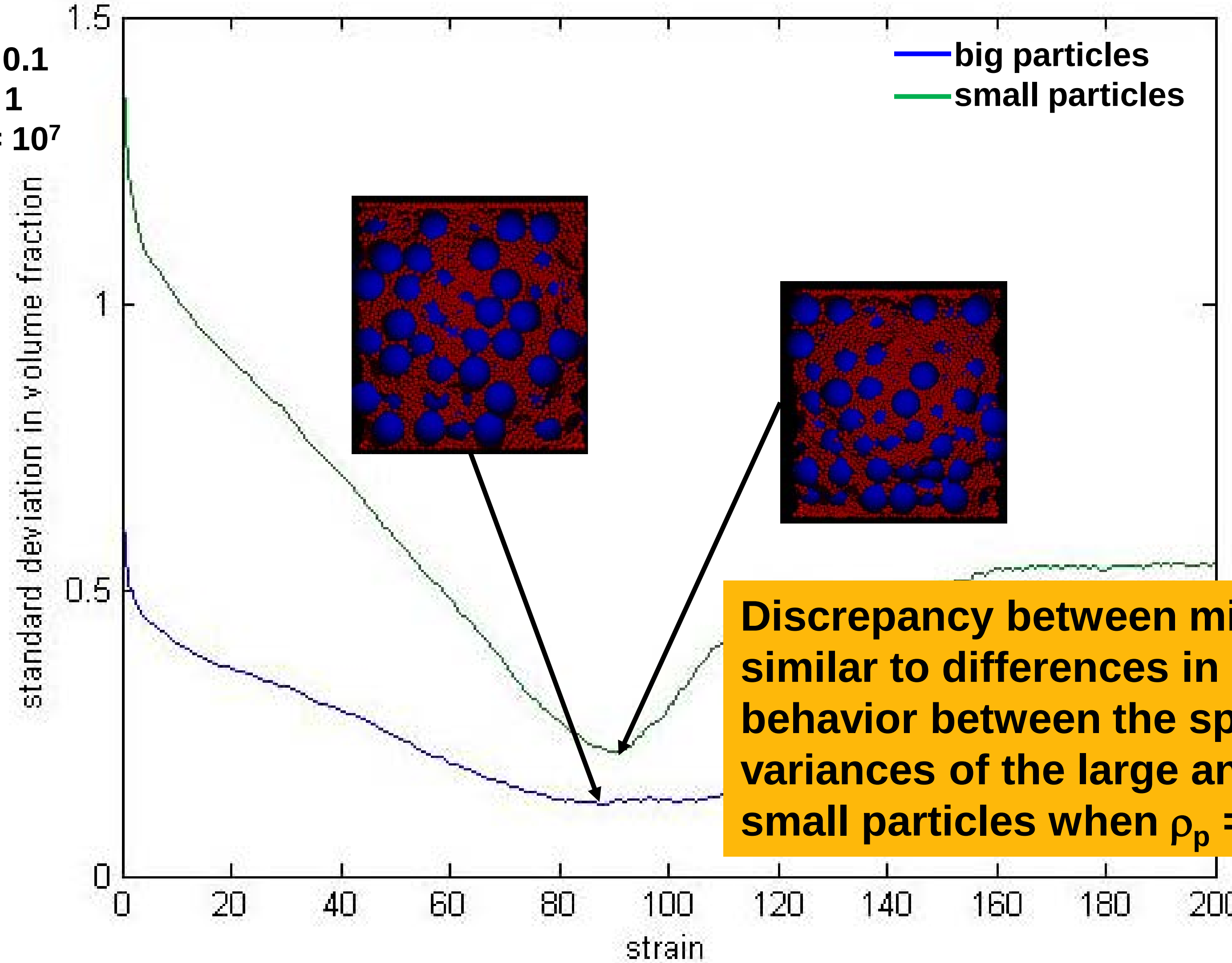
S = 0.1
B = 1
*k** = 10^7



But can the volume fraction be used as a good quantification of homogeneity?

Minima in the spatial variance in species concentration *may* also be used to identify and quantify well-mixed state

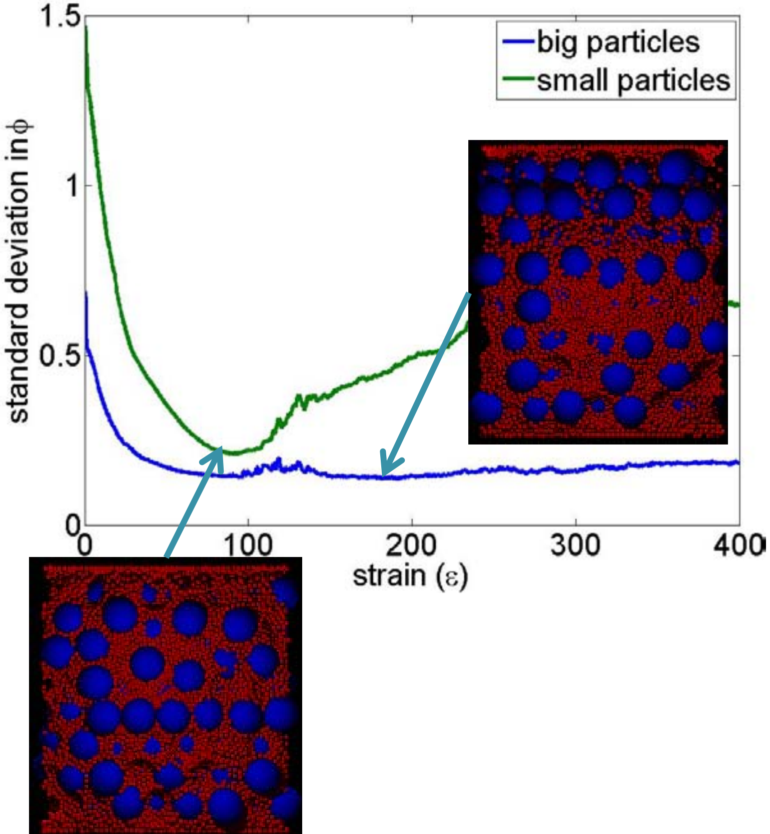
S = 0.1
B = 1
k^* = 10^7



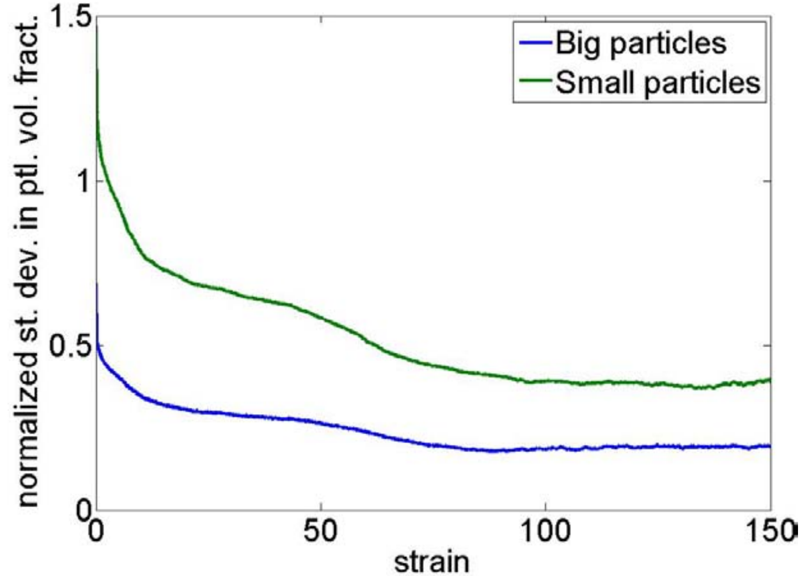
Discrepancy between minima similar to differences in behavior between the spatial variances of the large and small particles when $\rho_p = \rho_b$

However, minima in the volume fraction standard deviation may actually be achieved during un-mixing

S = 0.1
B = 0.1
$k^* = 10^6$



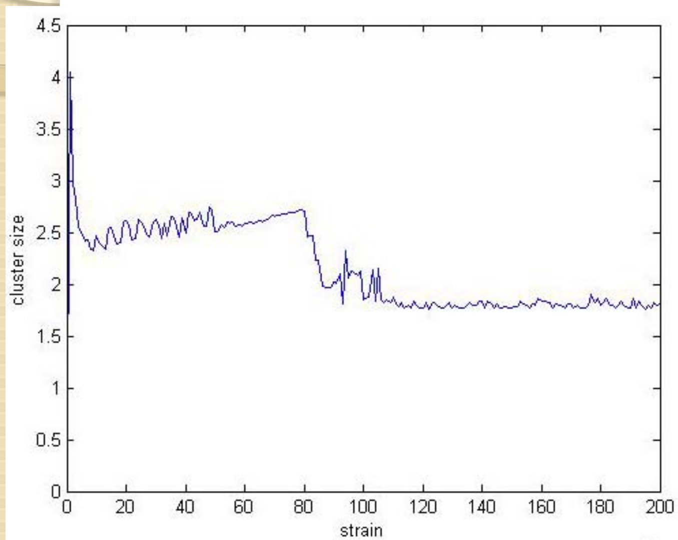
no cohesion
$k^* = 10^9$



Neither minimum well-defined

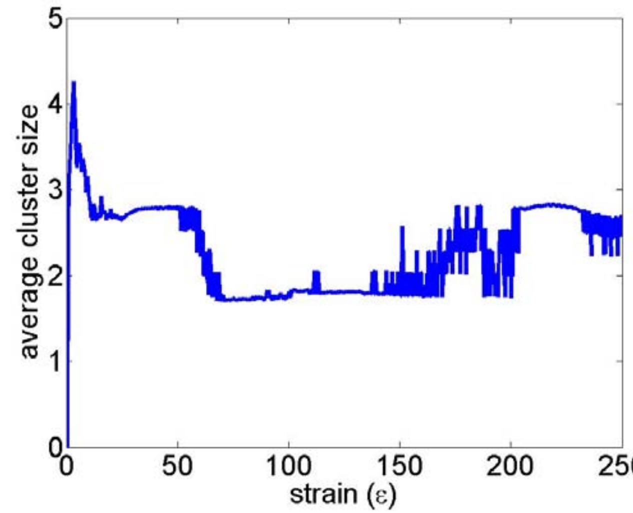
How useful is this statistic to identify and quantify homogeneous mixing?

The use of the average small-particle cluster size to identify and quantify homogeneous mixing is questionable

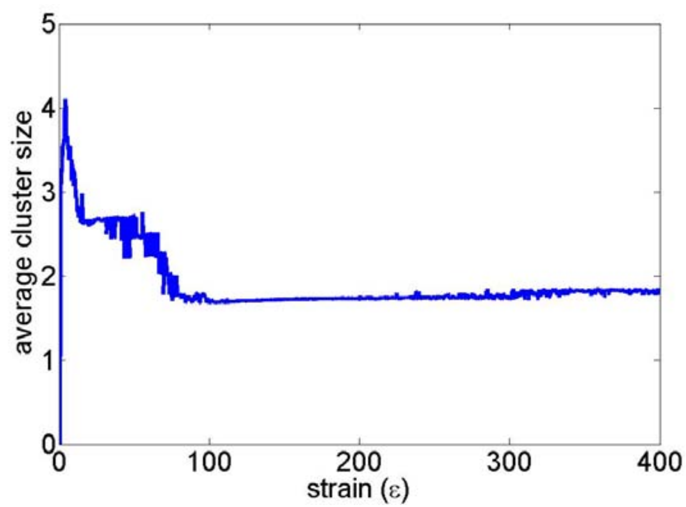


S = 0.1
B = 1
*k** = 10^7

no cohesion
*k** = 10^7



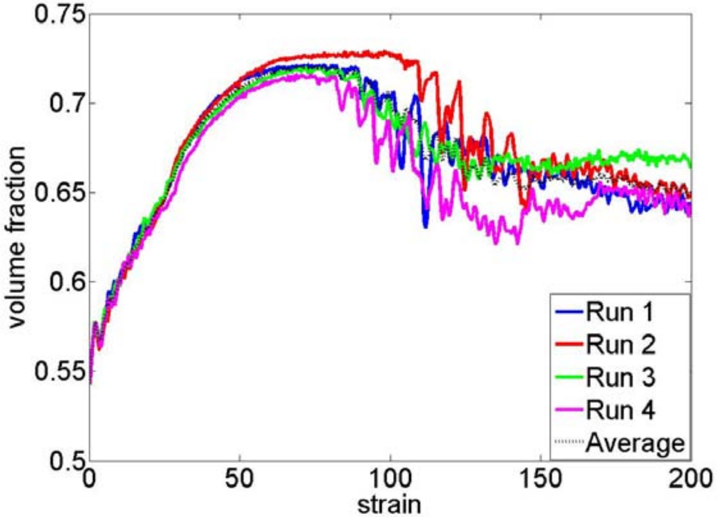
Minima are generally not well-defined and do not necessarily correspond to states of good mixing

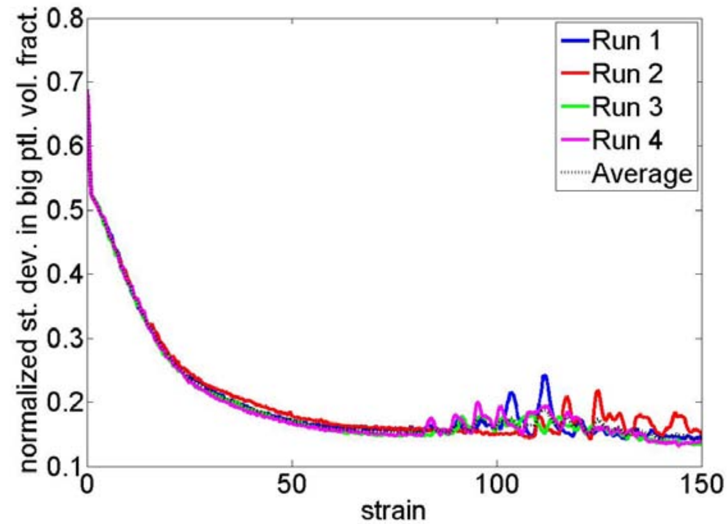


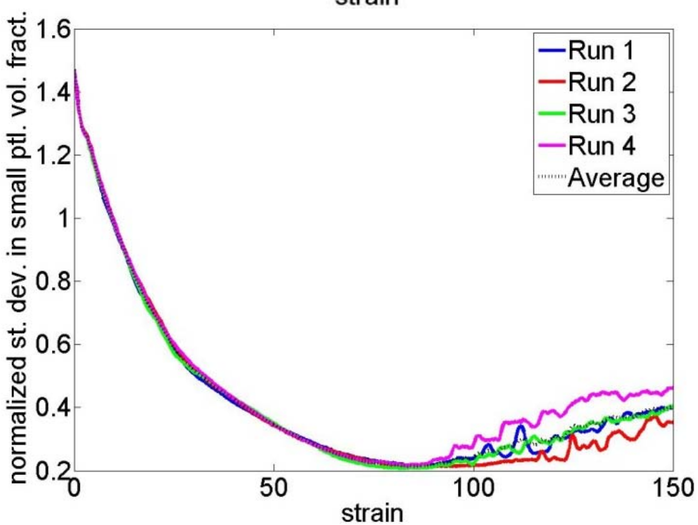
S = 1
B = 0.1
*k** = 10^6

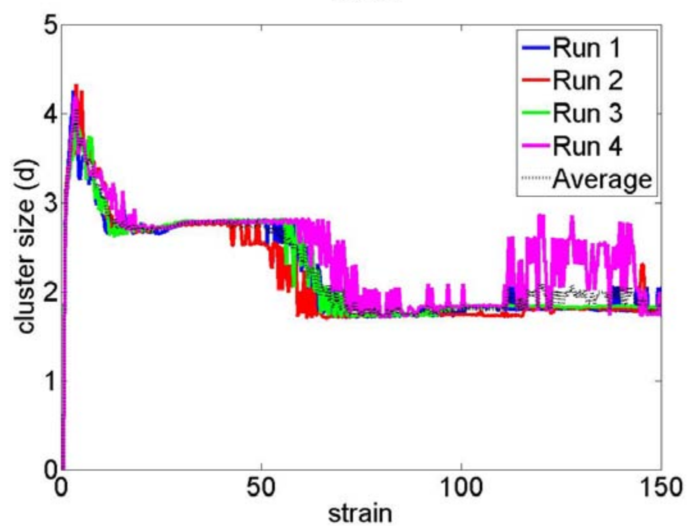
Initial conditions may affect *when* the most homogeneous mixtures are achieved, but not necessarily how homogeneous they are

no cohesion $k^* = 10^6$









Not enough simulations have been run at this time to describe a relation between homogeneity and cohesion and shear rate, but the results obtained so far suggest that it is complex and may be impossible to predict

Summary

- DEM simulations of bidisperse cohesive particles in the presence of an inviscid binder under shear were performed to determine how the homogeneity of the materials vary with the particle cohesiveness, mixing speed, and binder density
- When particles are neutrally buoyant in binder
  - Homogeneous mixtures are achieved when the shear rate is large or the small particles are not very cohesive
  - When the mixtures are inhomogeneous, they are less so when the big particles are as cohesive as the small ones
  - The volume fraction fails to capture the homogeneity as well as the other metrics which all display different behaviors
- When particles are denser than the binder (and particles are initially segregated vertically)
  - A spike in the volume fraction occurs when "good mixing" occurs, followed by un-mixing
  - The average cluster size and spatial variance in particle species concentration are not necessarily minimized when mixtures are visually homogeneous and so may not be the best way to quantify homogeneity
  - Initial conditions have a greater influence on the temporal evolution of the mixtures than on how homogeneous the mixtures become

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